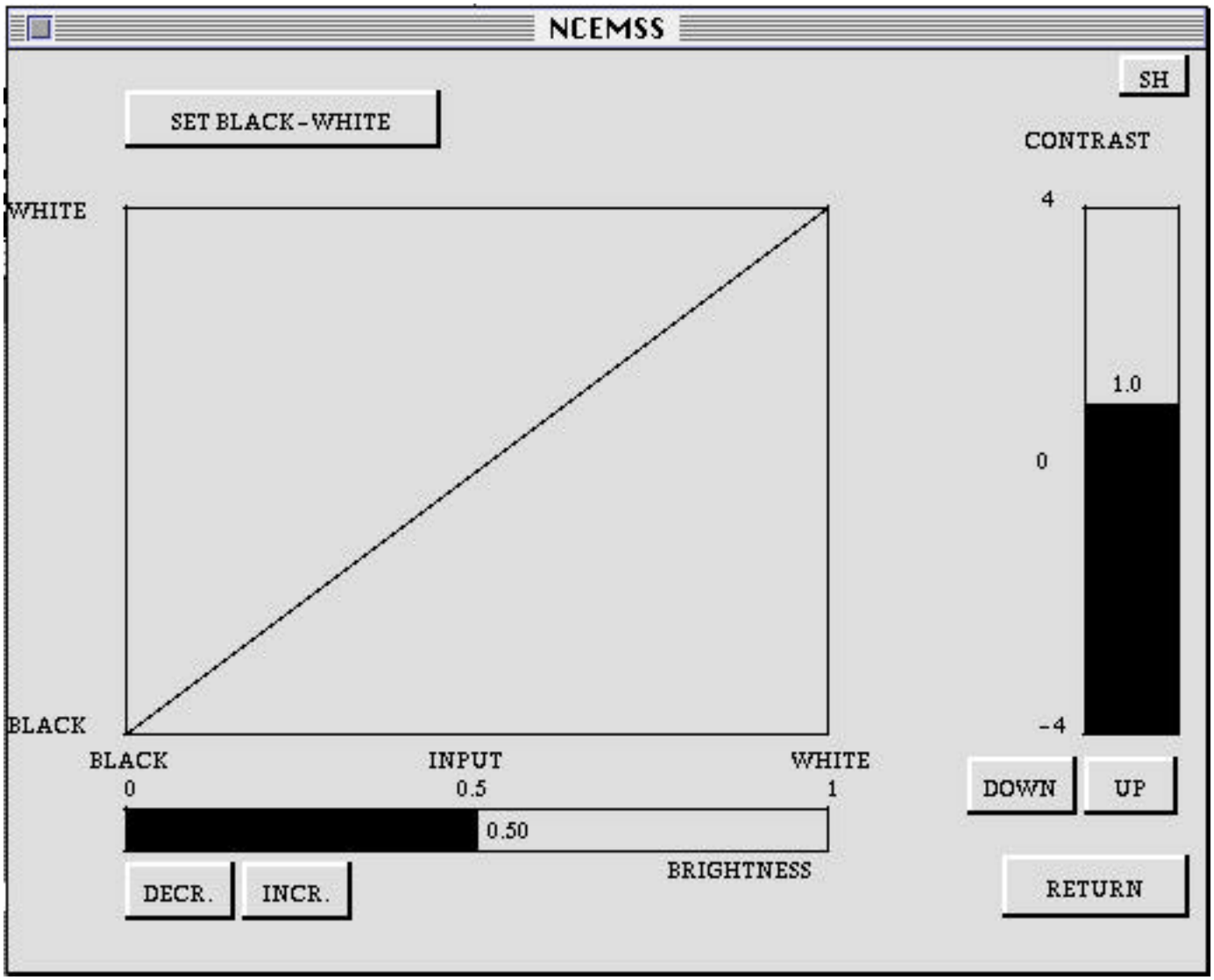
SET CAMERA LENGTH: is used to adjust the magnification of the diffraction pattern display. The value is input in mm., and has a default setting of 520mm.
INDEX DIFFR.PT.: is used to index a diffraction pattern. On moving the cursor to the selected diffraction spot and clicking the mouse, the indices are written next to the spot.
CHANGE CENTER OF DIFFR.PT.: The center of the displayed diffraction pattern can be changed by selecting this command and using the mouse to click on the desired position in the image display window.
READ THE CURSOR POSITION: reads the cursor position within an image.
ERASE THE DISPLAY: does just that.
WRITE TEXT ON THE DISPLAY: is used to write text at the cursor position.
STORE PARTS OF THE DISPLAY: after selecting this command, mark the corners of an area of the display window (image) to be stored and the image will be saved in a file. The user is prompted for a name and the program will automatically add the extension .at
DISPLAY STORED IMAGE: use this command to displayed a stored image of the type <name>.at created by the previous command.
PRINT STORED IMAGE FILE: sends the content of the file <name>.at to a connected laserprinter. The program creates a file "laserprinter.ps" and uses the command "lpr laserprinter.ps" to send the file to the printer. It is up to the user to set up the appropriate redirection of the output to a valid printer.
PRINT THE SCREEN: sends the content of the image window to a connected laserprinter. It otherwise works identical to the command above.
LIST STORED IMAGE-FILES: sends the command "ls *.im" to the operating system. The output list of stored image files is displayed in the terminal session window.
SET CONTRAST FOR LASERWRITER: allows the user to change the values of brightness (normally 0.5) and contrast (normally 1.0) of the printed image
SET DIV.ANGLE FOR DP: use this to change the size of the displayed diffraction spots in case the size is not optimal for viewing.
IMAGE ONLY<>OVERLAY ATOMS: controls whether atom positions are overlayed on the image or not.
AUTOSCALE-FIXED: use this to either let the computer choose black and white levels automatically or to use fixed values input by the user.
DISPLAY<>PRINT: in the display position, anything "DISPLAYED" goes to the image window. In the PRINT position, the actual numeric data is sent to a file in a format that depends on the setting of the switch ascii/binary below.
REL PHASE <> PHASE: determines if the phases reported for diffracted beams include the phasechange due to the mean inner potential of the crystal
ASCII FILE<>BINARY FILE: determines if the numeric output data for an image, projected potential or complex wavefunction is in ascii or binary.
OUT->PRINTER<>OUT->FILE: normally when you reroute the output to the printer, the program executes the command "lpr laserprinter.ps". Selecting OUT->FILE will create a named postscript file that can be saved and printed at any time later.
NORM.MONT<>CUSTOM: allows extra control on the layout of montaged images.

The Set Contrast Menu



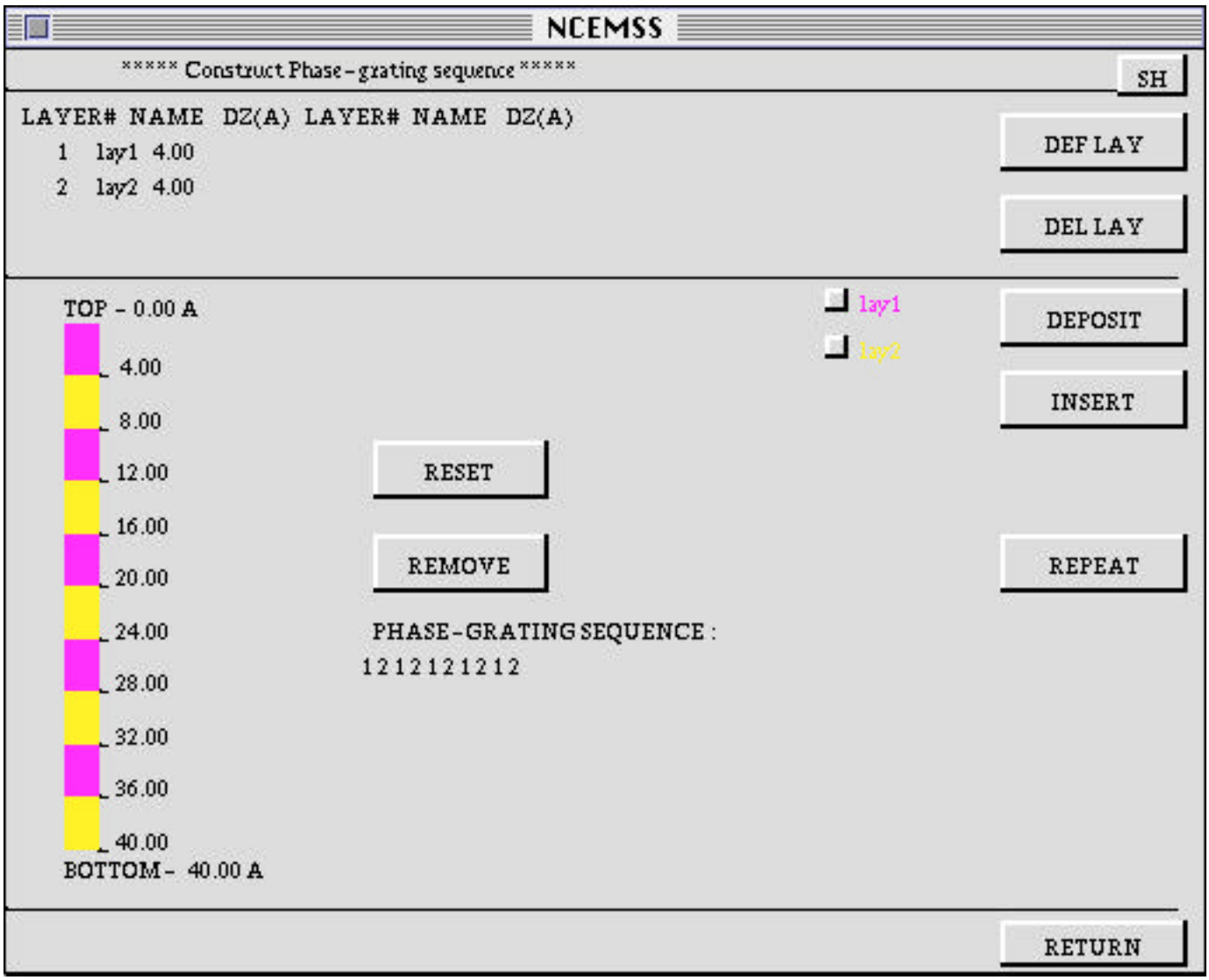
3.14 The SET-CONTRAST menu

When the ADJ.CNT box of the IMAGE-DISPLAY menu (page 38) is activated, it brings up the SET-CONTRAST menu. This menu displays the current contrast and brightness settings graphically. The straight line shows the mapping of the image intensity values (horizontal axis) into the displayed output intensity values (vertical axis). For a one-to-one mapping, the values of contrast (vertical bar-graph) and brightness (horizontal bar-graph) should be 1.0 and 0.5 respectively.

To increase (or decrease) the contrast used to display the image, tap the mouse with the cursor positioned over the UP (or DOWN) boxes underneath the vertical bar-graph. The contrast-transfer graph will pivot about its mid-point as the contrast is changed, providing a plot of how input grey levels are mapped into output greyscale levels. Note that a contrast value of less than zero will produce a negative image.

To increase (or decrease) the image brightness, use the INCR. and DECR. boxes to move the mid-point of the contrast-transfer graph to the left or right.

The contrast-transfer curve may be set directly, by activating the SET BLACK-WHITE box, then clicking the mouse after positioning the cursor at one end-point of the desired line, then clicking at the other endpoint. These end-points need not be exactly on the lines forming the box enclosing the contrast-transfer graph.


NCEMSS
***** Construct Phase-grating sequence *****
SH
LAYER# NAME DZ(A) LAYER# NAME DZ(A)
1 lay1 4.00
2 lay2 4.00
DEF LAY
DEL LAY
TOP - 0.00 A
4.00
8.00
12.00
16.00
20.00
24.00
28.00
32.00
36.00
40.00
BOTTOM - 40.00 A
lay1
lay2
DEPOSIT
INSERT
RESET
REMOVE
REPEAT
PHASE-GRATING SEQUENCE :
1212121212
RETURN

3.15 The SET-LAYERS menu

If the LAYERED STRUCTURE option is selected from the SINGLE/LAYERED menu (page 12), then the SET-LAYERS menu appears. This menu can be used to "construct" a specimen consisting of multiple layers of different single structures.

DEF LAY: To include a structure in the phase-grating sequence thatwill comprise the final layered structure, use the DEF LAY box and enter the name of the structure as it appears in the FILE-LIST menu (p.14). Up to six different structures may be used to make up the layered structure. Note that a PHSGRT calculation (p.21) must be carried out for any structure before it can be included in a layered calculation. Also note that, as well as existing, all the phase-gratings used to build a layered structure must be the same shape and size; i.e. each phase-grating must have the same values for the projected (two-dimensional) cell axes and cell angle, and also be computed out to the same scattering parameter, GMAX.

DEL LAY: This box is used to remove a previously-defined layer name from consideration.

DEPOSIT: The layered structure can be built up by depositing layers of any member structure that was defined earlier using DEF LAY. Each deposition is made by clicking on the DEPOSIT box, then on the appropriate LAYER symbol, then entering the layer thickness desired. The final structure is built from the top down; i.e. each subsequent layer is deposited onto the bottom of any existing sequence. A graphical repesentation of the structure appears on the left of the menu, and the phase-grating sequence is also listed.

INSERT: In addition to depositing a specified thickness of a chosen layer, it is possible to insert a specified thickness at any chosen thickness of the final structure. Clicking on this button, followed by the appropriate LAYER symbol, causes NCEMSS to ask for a layer thickness to be inserted, and the structure thickness at which to insert it.

REPEAT: This button is used to repeat a defined sequence a chosen number of times in order to build up a periodic layer structure.

RESET: This button zeros everything in preparation for another try.

REMOVE: The phase-grating sequence can be operated on directly to remove single slices, one at a time, by activating this button and clicking on the offending phase-grating in the sequence.

Appendix AMultislice Size, PhaseGrating Size, and Maximum G

The "size" of a multislice calculation is defined conveniently by the size of the largest array (the Q(k) or q(x) array). For an array size of 2nx2m, the multislice is said to be a "parameter n+m" multislice; thus a parameter-16 multislice will have a Q(k) array size of 256x256, (or 512x128, or 1024x64, or 2048x32, or 4096x16, depending upon the shape of the unit cell used in the computation). This size parameter must apply to all multislice programs, regardless of which of the three current algorithms (reciprocal-space, Fourier-transform, or real-space) is employed by the program.

A.1 Reciprocal-space multislice

As introduced by Goodman and Moodie (1974), the basic recursive form of the multislice description of dynamical diffraction can be written as

$$\Psi_{n+1}(\mathbf{k}) = [\Psi_n(\mathbf{k}) \bullet P_{n+1}(\mathbf{k})] * Q_{n+1}(\mathbf{k}) \qquad \text{(A1)}$$

That is, $\Psi_{n+1}(\mathbf{k})$, the wave function (given in reciprocal space) at the exit surface of the (n+1)th slice, is obtained by multiplying the wave function at the exit surface of the nth slice by $P_{n+1}(\mathbf{k})$, the propagator for the (n+1)th slice, followed by the convolution of this result by $Q_{n+1}(\mathbf{k})$, the phase-grating function (given in reciprocal space) for the (n+1)th slice.

In multislice computer programs that use the above reciprocal-space formulation, the three functions, $\Psi(\mathbf{k})$, $P(\mathbf{k})$, and $Q(\mathbf{k})$ are represented by two-dimensional arrays containing terms with indices that can be regarded as those of the diffracted beams within the diffracting specimen. In order to impose no extra symmetry on the computation, a "circular aperture" is usually placed on the terms in the arrays, so that terms beyond a certain distance in reciprocal space are set to zero. Note that the $Q(\mathbf{k})$ array must extend out to twice as far in reciprocal space as the $\Psi(\mathbf{k})$ and $P(\mathbf{k})$ arrays in order to correctly include all physical scatterings to each diffracted beam. Figure A1 shows how this doubled phase-grating requirement arises because $Q(\mathbf{k})$ is a "probability map" of terms that determine how much of each diffracted beam is to be scattered through the angle corresponding to the term. Thus, in order to compute the scattering of diffracted beams out to k = ±(h,k), the $\Psi(\mathbf{k})$ and $P(\mathbf{k})$ must be (2h+1)x(2k+1) in size, and Q(k) must be (4h+1)x(4k+1). For example, the SHRLI80 programs used a 128x128 array for $Q(\mathbf{k})$, making SHRLI80 a parameter-14 multislice and giving a maximum (h,k) value of (31,31); this limits the number of diffracted beams to less than 4096, adequate for most perfect-crystal computations, but too small for simulation of many defect structures (O'Keefe et al, 1978).

A.2 Fourier-transform Multislice

For larger arrays (and thus larger numbers of diffracted beams), it is faster to compute the multislice by recasting (A1) into a form where the convolution is replaced by two Fourier transforms and a multiply operation, as was done by early users of multislice in the Melbourne group. Then

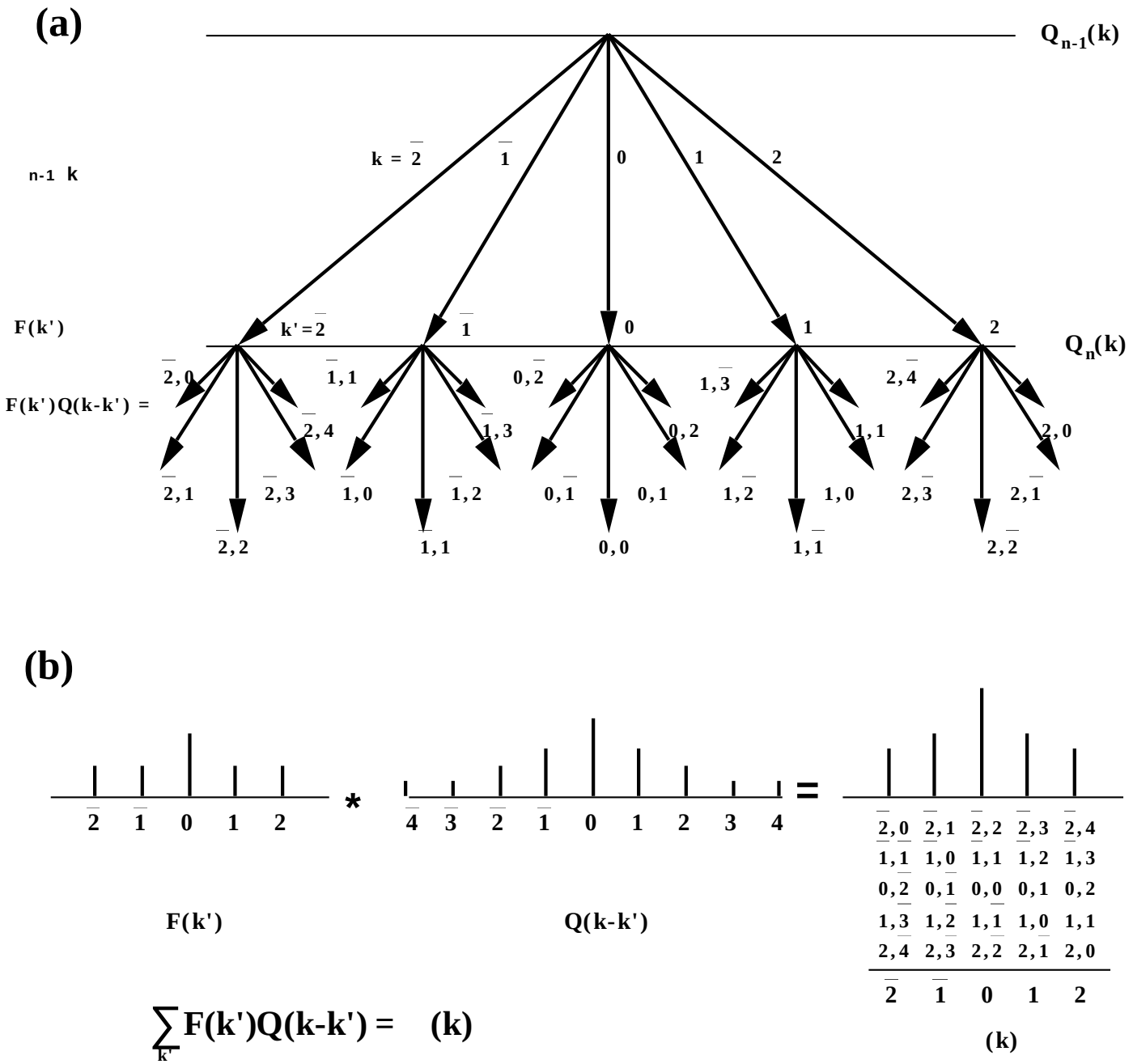


Fig. A1. Convolution description of multiple scattering. In order to include all scattering contributions to the dynamic electron wavefield Ψ(k), the phase-grating coefficients Q(k) must extend out twice as far in reciprocal space as do the coefficients of the wavefield. For the five depicted diffracted beams Ψ(k), (where |k|= -2,-1,0,1,2), the convolution requires nine phase-grating coefficients Q(k), (where |k|= -4 to 4).
(a) sketch of the contributions to the five diffracted beam directions; note that (e.g.) the contribution of the incoming Ψ(2) beam to the outgoing Ψ(-2) beam requires the presence of the Q(-4) phase-grating coefficient.
(b) Delta-function representation of the scattering process, showing each F(k').Q(k-k') term contributing to the outgoing Ψ(k), |k| = -2 to 2. Here the incoming function F(k) is equal to the product Ψ(k).P(k) in equation (A1). Note the presence of the Q(±3) and Q(±4) coefficients in the table of interactions; except for Ψ(0), every outgoing Ψ(k) contains a contribution from these outer coefficients, and would be in error without them.

$$\Psi_{n+1}(\mathbf{k}) = F\,[F^{-1}[\Psi n(\mathbf{k}) \bullet P_{n+1}(\mathbf{k})] \bullet q_{n+1}(\mathbf{x}) \qquad \text{(A2)}$$

Here the F represents the Fourier transform operation, and q(**x**) is the real-space form of Q(**k**), i.e. the (inverse) Fourier transform of Q(**k**). Experience with the SHRLI programs has produced the not-surprising result that, in order to obtain the same results with (A2) as with (A1), q(**x**) must be formed from a Q(**k**) that extends twice as far in reciprocal space as do Ψ(**k**) and P(**k**).

Note that, as well as correctly describing the physics of the scattering process by ensuring that all contributions from all the diffracted beams leaving the previous slice to each diffracted beam from the current slice are included, the doubled phase-grating also neatly eliminates the possibility of any "aliasing" arising from the necessary sampling of the real-space functions. Unfortunately, in their description of the FFT multislice, Ishizuka and Uyeda (1977) stated that the number of diffracted beams must be no less than the number of phase-grating coefficients; under their condition, the effects of aliasing will produce incorrect scattering results if array sizes are not made large enough to produce essentially zero electron amplitude over the outer five-nineths of the phase-grating and wave-amplitude arrays. This confusion appears to have arisen when the concept of FFT multislice was introduced to the Kyoto group by a visiting researcher familiar with its use in the Physics Department of Melbourne University. At Melbourne, it had been found that aliasing occurred when the convolution step of the reciprocal-space multislice (equation A1) was replaced by a forward/inverse Fourier transform sequence. This aliasing boosted the amplitudes of the outer beams in the calculation until "knock off" parameters were introduced to set the outer beam amplitudes to zero after each slice. However, even after this procedure eliminated the aliasing effect, results from the FFT multislice did not exactly match ones from the "standard" reciprocal-space formulation (O'Keefe, 1972). For this reason, the SHRLI80 programs (O'Keefe et al, 1978) continued to use the (slower) reciprocal-space form of the multislice. Experiments with various scattering algorithms (Self et al, 1983) led to the testing of different ways of avoiding aliasing in FFT multislice. It was realized that one such method was by choosing a q(x) formed from Q(k) terms that extended only 2/3 of the way to the array edges, provided that only the same number of diffracted beams was used in Y(k), with the outer 5/9 of the diffracted beam array reset to zero after every slice. A better method was to ensure that q(x) was formed from a Q(k) that extended out to twice the scattering angle as Ψ(k), and to reset the outer 3/4 diffracted beams to zero after each slice. This latter method conforms to the physics of the scattering process (fig.A1), and proved to yield the same results as the reciprocal-space multislice. A multislice program using this method was incorporated into the SHRLI81 suite, and this method is used in the NCEMSS multislice program (O'Keefe and Kilaas, 1988).

A.3 Real-space multislice

A third method of computing the multislice is to carry out the calculation completely in real space; this is an alternative to computing in reciprocal-space (as in equation A1), or in both real and reciprocal-space (as in equation A2). Fourier transformation of (A1) gives